DR-15. FULLERENE CHEMISTRY: A NEW REACTION FOR THE SYNTHESIS OF PERSPECTIVE SEMICONDUCTOR MATERIALS FOR ORGANIC ELECTRONICS

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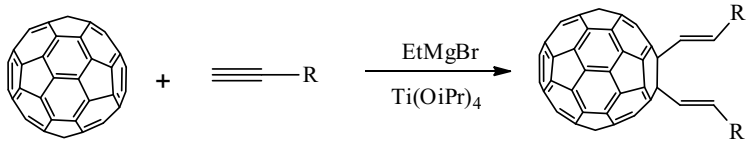
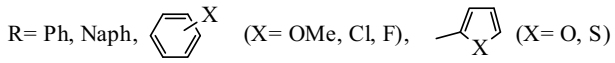
The report discusses the authors' original research aimed at developing new effective methods for the functionalization of carbon clusters in order to obtain previously difficult-to-access functionally substituted fullerenes that are promising as semiconductor materials for organic electronics.

Recently [1–7], we have designed efficient methods for direct functionalization of carbon clusters based on the reaction of C_{60} with carboxylic acid esters and nitriles, isonitriles and triazines in combination with EtMgX under the action of Ti complex. In continuation of this research, we have first studied the reaction between C_{60} and terminal acetylenes in the presence of EtMgBr and Ti(O*i*Pr)$_4$ to introduce conjugated aromatic and heteroaromatic addends into the C_{60} molecule.

It was found that the multicomponent reaction between C_{60} and aromatic or heteroaromatic terminal acetylenes in the presence of EtMgBr and Ti(O-*i*-Pr)$_4$ (chlorobenzene, 80 °C, 15 min, C_{60} : acetylene : EtMgBr : [Ti] = = 1 : 3 : 12 : 3) leads to acyclic fullerene bis-adducts, in which an aromatic or heteroaromatic substituent is attached to the fullerene core via a conjugated double bond. Terminal acetylenes containing saturated linear or cyclic substituents do not react with C_{60} under the same reaction conditions.





The results of preliminary theoretical studies indicate that solar cells created on the basis of such compounds will have a higher efficiency due to higher energy values of LUMO, as well as a smaller width of forbidden zone compared with devices based on PC [60] BM.

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